B.R.A Bihar University, Muzaffarpur

M.Phil. Sylllabus

Semester One:- Course work

		ESE	CIA	Total
Paper I	Research Methodology and computer application Chemical Research	70	30	100
Paper II	Theoretical Methods in Chemical Research	70	30	100
Candidates are required to choose any one paper. From the following				
Paper III (A)	Advances in Physical Chemistry Research	70	30	100
(B)	Advances in Inorganic Chemistry Research	70	30	100
(C)	Advances in Organic Chemistry Research	70	30	100

In each paper ten questions (two form each unit) to be set. The candidates are required to answer five questions (one from each unit). The duration of Term end Examination shall be 3 hrs.

Paper- I

Research Methodology and computer application Chemical Research

Unit-1 (a) Methods in Research

Objectives and importance of research, types of research, various stages of research viz identification of problem, characteristic of good, survey of literature, Research problem. Hypothesis formulation, research design, collection of data, analysis and interpretation, testing of hypothesis.

(b)Errors:

Sampling procedure of gases, solids and liquids, limitations of analytical methods, classification of errors, accuracy and precision, significant figures and computations

Unit-2 Research in Chemistry

(a) Introduction of national and international journals in chemistry, Rankling system of Journals and research papers, chemical abstracts, reviews, monographs and other resources in chemistry, IUPAC and its publication, national scientific bodies.

(b) Research communication: General aspect of scientific writing, writing literature4 survey and organising a poster display. Oral and Poster presentations, group discussion, short communication, component of research paper writing, writing of reviews and tertiary literature.

Unit-3(a) Safety and Ethics in Handling of Chemicals:

Ethics in chemical research, ethics in chfmical trading, classification and labeling of chemicals, storage of chemical, Hazardous chemicals, Use of Fume hoods in laboratories, sage handling and disposal of used chemical, Chemical waste treatment handling, shortage and waste disposal of radioactive chemicals.

(b)Statistics of Data Analysis:

Mean and standard deviation, reliability of result confidence test, T-text, and F-text, paired T test, correlation and regression, linear regression analysis of variance, Chi square test.

Unit-4 Basic of Computer & Information Technology:

History of computers, components of computer, primary and secondary memory, Hardware and Software, Binary number system and system and computation, RAM, ROM, Types of Operating System. Basic of Windows Operating System, Introduction of MS-Word, Excel and Powerpoint Presentation, Computer networking LAN, MAN, WAN, Internet and Types of World Wide Web. Study of information available at different websites of chemical importance.

Uint-5 Programming Languages:

Some useful Software of Chemical interest.

Paper-II

Theoretical Methods in Chemical Research

Unit-1 Quantum chemical methods I:

Postulates of quantum mechanics, atomic orbials of hydrogen and hydrogen like atoms, multi electron atoms, spin orbitals, self consistent field approximation.

Unit-2 Quantum chemical methods II:

(a) Molecular orbitals, Huckel molecular orbitals for ethylene, cyclobutadiene and butadiene.
(b) Theory of angular momentum, Angular momenta of composite system, Energy states and term symbols for atom and ions, Atomic spectra, effect of spin orbit interaction and crystal fields, Molecular term symbols for diatomic molecules.

. Unit-3 NMR Spectroscopy:

Basic Principles and instrumentation, chemical shifts and its measurements, coupling constants, peak area and intensity ratio, relaxation time, Double resonance technique, Application of NMR spectroscopy in structure determination of organic molecules, coordination compounds and ^{13}C nmr spectroscopy.

Unit-4 Infrared and Raman Spectroscopy:

(a) Basic principles and instrumentation, theory of Raman spectroscopy, Molecular vibrations (Fundamentals), overtones, combination bonds, selection rule ir and Raman active modes. Example of di, tri and tetra atomic molecules.
(b) IR spectra of SO^{2}_{4}, CO^{2-}_{3} and NO^{-}_{3} ion. Studies on coordination of CO^{2-}_{3} and CHCOO ion, application of ir spectroscopy to identify donor sites of a ligand such as thiourea, dithiocarbameates, thiocynates and isothiocynates, ir spectra of metal carbonlyls.

Unit-5 UV and IR spectroscopy of Organic compounds:

(a) Types of electronic transitions, selection rules for electronic transition, bathochromic and hypsochromic shifts, different types of chromophones, Woodward Fiser rule.
(b) Finger printing regions in IR Spectroscopy, Characteristic group frequencies, Interpretation of spectra, Electronic effects and IR frequencies Characteristic IR Spectra of organic molecules.

Paper III (A)

Advances in Physical Chemistry Research

Unit -1: introduction of Molecular dynamics and statistical thermodynamics

(a) Reaction pathways, Kinetic parameters. Mechanism of some oscillatory reaction
(b) Thermodynamic probabilities Boltzman distribution laws

Unit-2: Quantum mechanical calculation of molecular orbital:

Group theoretical methods for calculation of molecular orbital of benzene, cyclopentadienyl anion and naphthalene, Sine formula and its application.

Unit-3 Solid States :

Electrcal, optical, magnetic, thermal and mechanical properties, magnetic materials, mixed oxide, semiconductor and super conductor

Unit-4 Photo physical Process:

Types of photo physical pathways, radiative transitions, Internal conversion and intersystem crossing, fluorescence, delayed fluoresce, excited state quenching, excimers and exciplex photo dimensation and photo redox reaction, phosphorescence and chemiluminiscence.

Unit-5 Surface Analytical Techniques :

(a) AES: Auger electron spectroscopy, electronic structure-isolated atoms, solid state ionization relaxation and anger emission.
(b) Low energy electron diffraction: basic theory, pseudo 2D structure.
(c) Elector energy Loss spectroscopy: Elastic Peak, selection rule, Molecular adsorption of CO on metallic surfaces.

Paper III (A)

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Paper III (C)

Advances in Organic Chemistry Research

Unit -1: Photochemical Reaction

Molecular orbitals, Fontier orbitals, general rule for periicylic reaction. Norrish type I and Norrish type II reaction, Thermal generation of excited states, photochemical rearrangements.

Unit-2: Synthesis and Spetral behavior

Studies on chloroquine, femotidine~~ranitidine~~ and cimetidine

Unit-3: Electrocyclic Reactions:

Thermal electrocyclic, photochemical electrocyclic metal catalysed electrocyclic reaction.

Unit-4: New trends in green chemistry

Basic principles of green chemistry dimethylcarbonate as green reagents, methods used in Green chemistry, synthesis of styrene, adipic acid, paracetamol and citral involving green chemistry

Unit-5: Steriochemistry

Discussion on the ~~biphenyl~~ compounds and nitrogen comporids